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SEARCH FOR BROKEN SYMMETRY IN THE Au(110) SURFACE

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Spin polarized LEED results are presented which confirm predicted symmetry induced properties. Contrary to recent claims, the results do not provide any evidence for a broken bulk derived symmetry in the Au(110) surface.

MEASUREMENTS of electron spin effects in *L*ow *E*nergy *E*lectron *D*iffraction (LEED) experiments provide additional observables from which emerge powerful conclusions with respect to crystal surfaces [1, 2]. In general, two types of electron spin polarization (ESP) experiments can be performed. The ESP of a diffracted beam (characterized by the wave vector **k** and the surface reciprocal net vector **g**) is obtained for unpolarized incident electrons (characterized by the wave vector $\mathbf{k}_0$) by measuring the components of the polarization vector $\mathbf{P}(\mathbf{k}_0, \mathbf{k}, \mathbf{g})$. Alternatively, the components of the corresponding asymmetry vector $\mathbf{A}(\mathbf{k}_0, \mathbf{k}, \mathbf{g})$ are obtained using suitable polarized incident electrons and are given by the normalized intensity changes of the observed LEED beam **g** as the polarization of the incident electron beam is reversed. For the vectors **P** and **A** it has been shown theoretically that their magnitudes P and A are equal [1, 3, 4]. **P** and **A** are both axial vectors, they therefore transform as axial vectors under rotation and reflection [3–5]. Further, for two diffraction processes time reversed to each other, and characterized by $\mathbf{k}_0, \mathbf{k}, \mathbf{g}$ and $-\mathbf{k}, -\mathbf{k}_0, -\mathbf{g}$, respectively, it follows $\mathbf{P}(-\mathbf{k}, -\mathbf{k}_0, -\mathbf{g}) = -\mathbf{A}(\mathbf{k}_0, \mathbf{k}, \mathbf{g})$ [6]. In addition, if the scattering plane (defined by $\hat{\mathbf{p}}_n = \mathbf{k}_0 \times \mathbf{k}/|\mathbf{k}_0 \times \mathbf{k}|$) coincides with a mirror plane of the crystal, **P** and **A** are always identical. Further, if the surface normal $\hat{\mathbf{n}}$ is a twofold rotation axis of the crystal, the components of **P** and **A** perpendicular to $\hat{\mathbf{n}}$ are equal for all specular beams $[\mathbf{g} = (0, 0)]$.

Here, we present spin polarized LEED results for the components $P_n = \mathbf{P} \cdot \hat{\mathbf{p}}_n$ and $A_n = \mathbf{A} \cdot \hat{\mathbf{p}}_n$ of **P** and **A** perpendicular to the scattering plane obtained from the (1×2) reconstructed Au(110) surface. They support theoretical predictions and they show that in the surface reconstruction of Au the 2-dimensional surface symmetry derived from the bulk (110) planes is not necessarily broken, contrary to recent claims drawn from experiments using the same techniques [7].

In this experiment instead of $\mathbf{k}_0, \mathbf{k}$, the beam energy E, the azimuth ϕ, and the scattering angle $\theta = \measuredangle(\mathbf{k}_0, \mathbf{k})$ are used to describe the diffraction. The scattering plane always contains the surface normal $\hat{\mathbf{n}}$. ϕ is the angle between the trace of the scattering plane in the surface and the $[1\bar{1}0]$ closed packed chains of the surface.

In Fig. 1, $P_n(\theta)$ profiles, measured at fixed energy $E = 50$ eV, are shown for two 00 beams time reversed to each other, and with the scattering plane not a mirror plane of the crystal (azimuth $\phi = 35°$). With the (positive) sign referred to $\hat{\mathbf{p}}_n = \mathbf{k}_0 \times \mathbf{k}/|\mathbf{k}_0 \times \mathbf{k}|$, $P_n(\theta)$ should be identical for both beams if the surface has the twofold rotation axis of the bulk. Indeed, both profiles are in good agreement, and therefore, $P_n(\theta)$ and $A_n(\theta)$ should also be identical. In an earlier work [7], however, a disagreement between $P_n(\theta)$ and $A_n(\theta)$ was found for the same scattering plane and the same LEED beam, and was taken as evidence for broken symmetry. We believe that this discrepancy stems from the strong sensitivity of $A_n(\theta)$ [7] and, therefore, of $P_n(\theta)$ to the azimuth ϕ, connected with misalignments and with disturbances by stray magnetic fields.

Further symmetry operations on $P_n(\theta)$ are shown

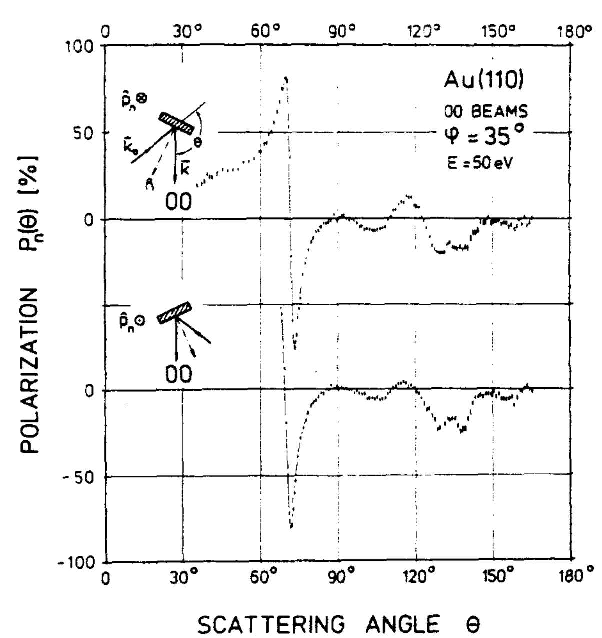

Fig. 1. $P_n(\theta)$ profiles for 00 LEED beams from Au(110) reversed to each other. The scattering energy is $E = 50 \pm 1$ eV, the azimuth $\phi = 35 \pm 2^\circ$ (scattering plane is not a mirror plane of the bulk). The error bars give the statistical errors due to the counting in the Mott detector. Additional errors are: polarization zero: ± 1%, calibration of polarization: ± 5% of given values, absolute value of scattering angle θ: ± 3°, changes in θ: ± 0.3°. Note that in the laboratory system P_n change the sign under time reversal ($\hat{\mathbf{p}}_n \to -\hat{\mathbf{p}}_n$).

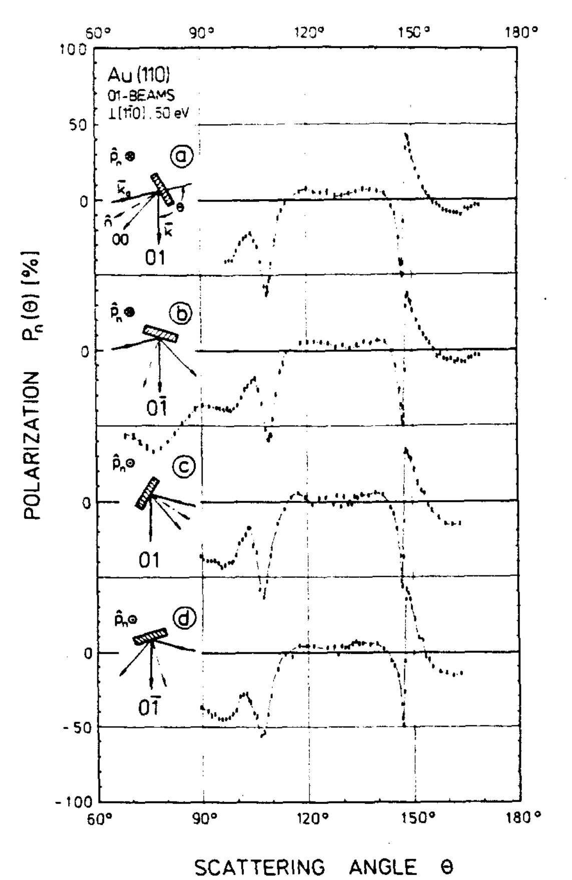

Fig. 2. $P_n(\theta)$ profiles for the 01 and 0$\bar{1}$ LEED beams from Au(110). The scattering plane is the (1$\bar{1}$0) mirror plane of the bulk ($\phi = 90 \pm 2^\circ$, perpendicular to the close-packed chains of the (110) plane) and $E = 50$ eV. For experimental errors see Fig. 1.

in Fig. 2 for 01/0$\bar{1}$ beams at $E = 50$ eV. Here, the scattering plane is a mirror plane of the crystal. The insets show each scattering condition for which the $P_n(\theta)$ for the set of 01/0$\bar{1}$ beams are obtained [8, 9]. Operations (a) into (c) and (b) into (d) represent a reflection at the plane ([1$\bar{1}$0] x k) defined by [1$\bar{1}$0] and **k**. Therefore, in the laboratory system for (c) and (d) $\hat{\mathbf{p}}_n$ is antiparallel to that for (a) and (b). A combined operation, consisting of a time reversal, a reflection at the plane ([1$\bar{1}$0] x k), and a rotation around [1$\bar{1}$0] transforms (a) into (b) and (c) into (d), as seen from the insets [9]. The excellent reproduction of the $P_n(\theta)$ profiles under all these spatial symmetry operations and under the time reversal confirms the theoretical results [1, 3, 4] and does not show a broken bulk derived symmetry at the (1 x 2) reconstructed Au(110) surface.

For a 0$\frac{1}{2}$ beam measured at the energy $E = 50$ eV with the [1$\bar{1}$0] mirror plane of the bulk being the scattering plane, a lack of agreement between $P_n(\theta)$ and $A_n(\theta)$ was also found and interpreted as a broken bulk derived symmetry at the surface [7]. These results were then used to exclude all models of Au(110) (1 x 2) surface reconstruction with a mirror symmetry perpendicular to the close-packed [1$\bar{1}$0] chains. This claim is incorrect due to the doubtful reliability of the corresponding measurements [7]. Figure 3 illustrates $P_n(\theta)$ profiles (a, b) and $A_n(\theta)$ profiles (c, d) for the 0$\frac{1}{2}$ and 0$\bar{\frac{1}{2}}$ beams at $E = 50$ eV, with the scattering plane being the (1$\bar{1}$0) mirror plane of the bulk. As is apparent from Figs. 3(a) and 3(b), measurements of $P_n(\theta)$ for the 0$\bar{\frac{1}{2}}$ beam are in agreement with those for the 0$\frac{1}{2}$ beam performed under identical scattering conditions.

Like the $P_n(\theta)$ profiles for the 01 and 0$\bar{1}$ beams [Figs. 2(a, b)], those for the 0$\frac{1}{2}$ and 0$\bar{\frac{1}{2}}$ beams [Figs. 3(a, b)] are related to each other by a time reversal and a reflection at the plane ([1$\bar{1}$0] x k). Hence, the agreement of $P_n(\theta)$ for both beams places a doubt on the earlier conclusions [7]. Figures 3(c) and 3(d) shows the corresponding $A(\theta)$ profiles for the same 0$\frac{1}{2}$ and 0$\bar{\frac{1}{2}}$ beams obtained in an apparatus described earlier [10]. These $A_n(\theta)$ profiles from both beams are not only identical to each other, but are also in good agreement with the $P_n(\theta)$ profiles (Fig. 3). It is difficult to imagine the origin of the erroneous results reported in [7].

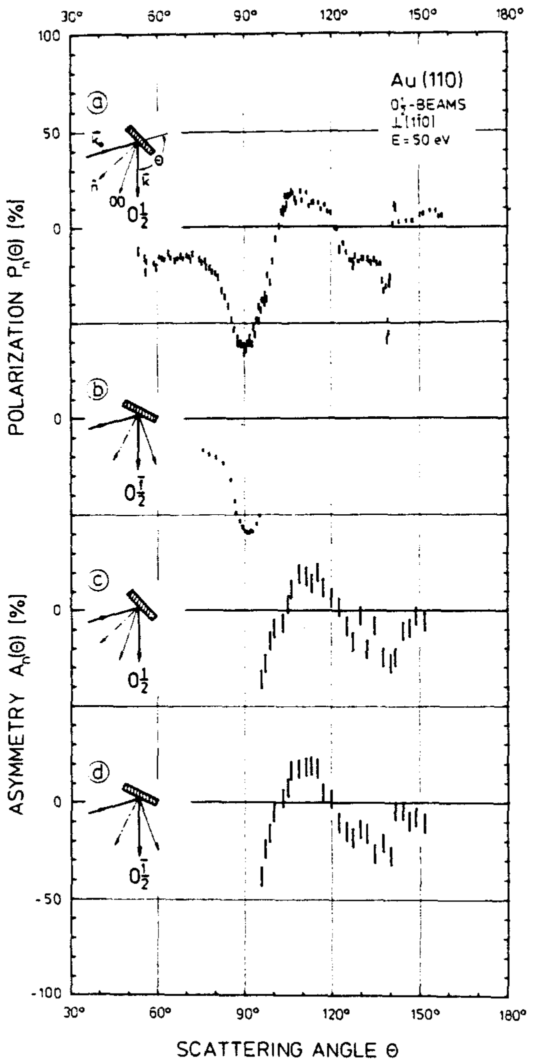

Fig. 3. $P_n(\theta)$ profiles (a, b) and $A_n(\theta)$ profiles (c, d) for the $0\frac{1}{2}$ and $0\frac{\bar{1}}{2}$ LEED beams from Au(110) for $E = 50$ eV. The scattering plane is the $(1\bar{1}0)$ mirror plane of the bulk ($\phi = 90 \pm 2°$). For the experimental errors in $P_n(\theta)$ see Fig. 1. The error bars for $A_n(\theta)$ give estimated errors due to the zero instability of the current meter. The absolute values of $A_n(\theta)$ are fitted to $P_n(\theta)$. The errors in angles are similar to those of $P_n(\theta)$.

Because ESP in LEED is sensitive only to averaged scattering properties of small areas of multiple scattering [11] the results presented here allow statements only about the symmetry of an "averaged surface". Averaged symmetry properties of the surface, e.g. for a domain structure, are governed by the symmetries of the bulk (110) planes. Therefore, any broken bulk derived surface symmetry in experimental results would be difficult to comprehend. In addition, all areas of multiple scattering which contribute partial waves to the half order beams, also contribute waves to the integer order beams. Therefore, in constrast to earlier conclusions [7], the symmetry properties of the surface are present in the integer order beams as well as in the half order beams.

Taken together the $A_n(\theta)$ profiles obtained with a GaAs source of polarized electrons, together with the different $P_n(\theta)$ measurements presented here do not suggest any broken bulk derived symmetry in the (1 x 2) reconstructed Au(110) surface.

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REFERENCES

1. R. Feder, *J. Phys.* **C14**, 2049 (1981).
2. D.T. Pierce & R.J. Celotta, *Adv. Electron. Electron Phys.* (Edited by C. Marton), Vol. 56. Academic Press, New York (1981).
3. R. Feder, *Phys. Lett.* **78A**, 103 (1980).
4. B.I. Dunlap, *Solid State Commun.* **35**, 141 (1980).
5. P. Bauer, R. Feder & N. Müller, *Solid State Commun.* **36**, 249 (1980).
6. This follows by inserting in Ref. [3], equation (4) into equations (1), (2) and (3).
7. B. Reihl & B.I. Dunlap, *Appl. Phys. Lett.* **37**, 941 (1980); B. Reihl, *Z. Physik* **B41**, 21 (1981) and Ref. [1] therein.
8. Experimental details: see R. Feder, N. Müller & D. Wolf, *Z. Physik* **B28**, 265 (1977) and [9].
9. N. Müller, Dissertation München (1977); N. Müller, Report 9/23, MPI für Plasmaphysik, Garching (1979).
10. M. Erbudak & H.C. Siegmann, *Satellite Conf. 10th Int. Conf. Phys. of Electronic and Atomic Collisions* (1977) (unpublished); M. Erbudak, *ZAMP* **29**, 347 (1978).
11. N. Müller & D. Wolf (to be published).